Stereochemistry

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Review 2-D Drawings

- Lines are bonds
- Hydrogens are assumed
- Saturated carbons at ends and corners unless otherwise specified
- Carbon bonded to OH
Review 2-D Drawings

3-D Drawings

3-D drawings more accurately represent bond angles, molecular shape, and differentiation of isomers.

Does not illustrate shape or bond angles.
3-D Drawings: Bonds

- Normal Bond
- Wedged Bond
- Dashed Bond

Bonds directed away from the viewer

Bonds in the plane of the page

Bonds directed toward from the viewer

3-D Drawings: More examples

- HOOC
- COOH
- CH₃
- H
- OH
- Cl
- Br
- HO
- OH
- OH
- H
Stereochemistry

Stereochemistry is the study of spatial properties of molecules that have the same formula and connectivity but have different 3-D shapes.

Stereoisomers are molecules with identically connected atoms but oriented differently in space.

Chiral Molecules

Entantiomers are stereoisomers which are mirror images of each other.

Chiral molecules are nonsuperimposable stereoisomers on their mirror. (ie, they show “handedness”.)
Examples of Chirality

Chiral Molecules

Achiral Molecules

Chiral Centers

**Chiral centers** are atoms, where the interchanging of any two bonds will result in the formation of a different stereoisomer.
Chiral Centers

Chiral Molecules

Achiral Molecules

Chiral Center Configuration

• Each chiral center has 2 possible configurations: R or S
• Rules for determining configuration:
  1. Assign each substituent a priority from 1 to 4 based on the following rules:
     A. Higher atomic number = higher priority
        I > Br > Cl > F > O > N > C > H
     B. If two atoms have the same atomic number, priority is determined by the “secondary” substituents
     C. If there are double or triple bonds on the secondary substituents, they are treated as 2 or 3 bonds.
Chiral Center Configuration

2. Orient the center such that priority number 4 is directed into the page

3. Determine R or S configuration by the direction of decreasing priority (increasing number)
   - Priority increases clockwise - R configuration
   - Priority increases counterclockwise, S configuration

Example of Chiral Center Configuration Determination
Multiple Chiral Centers

If a molecule has multiple chiral centers, this does not mean its chiral.

Any molecule with a plane of symmetry is achiral.

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Diastereomers

Diastereomers are pairs of molecules with more than one chiral center that are not mirror images of each other.

These molecules would be considered enantiomers if all chiral centers were opposite.

If this bond were directed toward the viewer, these would be enantiomers.
Examples of Diastereomers

Conformational Isomers

• Double bonds result in rigid structure, preventing bonds from changing conformation.
• If both carbons contain two substituents, two formations are possible:
  – Cis- “same side”
  – Trans- “opposite side” – add pictures
Comformation Isomers

Cis

Trans